

2-(P-nonylphenoxy)-6-benzyl pyrazine

Inchi:	InChI=1S/C26H32N2O/c1-2-3-4-5-6-7-9-12-22-15-17-25(18-16-22)29-26-21-27-20-24(28
InchiKey:	PJHZIBWEHBLJKC-UHFFFAOYSA-N
Formula:	C26H32N2O
SMILES:	CCCCCCCCc1ccc(Oc2cncc(Cc3ccccc3)n2)cc1
Mol. weight [g/mol]:	388.55
CAS:	116295-69-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.47		Crippen Method
logp	7.153		Crippen Method
mcvol	331.750	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116295693&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/93-107-0/2-P-nonylphenoxy-6-benzyl-pyrazine.pdf>

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